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The need for realistic simulations of phonon intensities in inelastic neutron and x-ray scattering – an experimentalist's perspective

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The advent of inelastic neutron scattering in the middle of the last century enabled detailed studies of lattice vibrations, i.e. phonons, in condensed matter. Initially focused on simple structures [1,2], inelastic neutron scattering has been instrumental for our understanding of superconductivity in A15 compounds [3] and more recent conventional superconductors [4,5]. However, many materials of current interest have a large number of atoms in the crystallographic unit cell, which results in an even larger number of phonon dispersion lines. Having obtained a data set from inelastic neutron or x-ray scattering, the experimenter relies heavily on model calculations for an understanding of the observed intensities. Naturally, such calculations become more demanding or even impossible with large unit cells.

Here, I will discuss various investigations of lattice dynamical properties by inelastic neutron and x-ray scattering in which ab-initio and other model calculations have been indispensable for a detailed understanding. I will highlight the way in which model calculations have been employed but also point out limitations. Finally, I will discuss based on these examples the need for more realistic simulations of phonon intensities requiring an improved link between lattice dynamical modelling and the experimental setup, i.e., evaluating resolution effects on the calculated phonon dispersion and intensities.

[1] B. N. Brockhouse and A. T. Stewart, Physical Review 100, 756 (1955).
[2] B. N. Brockhouse, K. R. Rao, and A. D. B. Woods, Physical Review Letters 7, 93 (1961).
[3] J. D. Axe and G. Shirane, Physical Review Letters 30, 214 (1973).
[4] F. Weber et al., Physical Review Letters 109, 057001 (2012).
[5] F. Weber, L. Pintschovius, W. Reichardt, R. Heid, K. P. Bohnen, A. Kreyssig, D. Reznik, and K. Hradil, Physical Review B 89, 104503 (2014).

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